**Amendment to the Claims:**

This listing of claims will replace all prior versions, and listings, of claims in the application:

**Listing of Claims:**

1. (Currently Amended) A computer system comprising:

a first database containing, records corresponding to a plurality of chemical compounds and records corresponding to biological information related to effects of such chemical compounds on biological systems;

a second database containing records corresponding to a plurality of molecular targets;

a third database containing records corresponding to screening results from *in vitro* assays measuring interactions between each of a plurality of compounds in the first database and each of a plurality of molecular targets in the second database, the results including information on the effect that a compound selected from the first database has on the interaction between a reference compound known to interact with a selected molecular target from the second database and said selected molecular target; ~~and~~

a user interface allowing a user to ~~view the selected compound and to selectively view information from the first database, the second database, and the third database as it relates to a compound record in the first database or as it relates to a molecular target in the second database~~provide the system with information about a new chemical compound; and

a query script that extracts information from the three databases that is relevant to the predictability of the potential use of the new compound as a drug.

2. (Original) The computer system of claim 1, wherein the interaction includes binding and the effect includes inhibitory effect.

3. (Previously Presented) The computer system of claim 1, wherein the chemical compounds include compounds with known biological activity.

4. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include compounds that have been or are being tested in preclinical studies in animals.

5. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include compounds known to have an effect on the environment.

6. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include pharmacological reference agents.

7. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include known pharmaceuticals in the market for clinical use for which there is a substantial amount of biological information available.

8. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include drug candidates approved by the Food and Drug Administration for testing in humans.

9. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include compounds obtained from natural sources that exhibit biological activity.

10. (Original) The computer system of claim 1, wherein the molecular targets include receptors.

11. (Withdrawn) The computer system of claim 1, wherein the molecular targets include enzymes.

12. (Withdrawn) The computer system of claim 1, wherein the molecular targets include nucleic acids.

13. (Withdrawn) The computer system of claim 1, wherein the molecular targets include carbohydrates.

14. (Original) The computer system of claim 1, wherein the records of the first database corresponding to a plurality of chemical compounds are organized in categories related to the description and properties of the compounds.

15. (Original) The computer system of claim 14, wherein the categories include:
compound name;
compound type;
physical-chemical characteristics;
chemical space coordinates or structural descriptors; and
solubility.

16. (Original) The computer system of claim 1, wherein the first database includes a natural product database.

17. (Previously Presented) The computer system of claim 1, wherein the first database includes a database of chemical compounds that have failed in preclinical or human clinical tests.

18. (Original) The computer system of claim 1, wherein the first database includes a chemical registry database.

19. (Original) The computer system of claim 1, wherein the second database includes a three-dimensional structure database.

20. (Original) The computer system of claim 1, wherein the second database includes a sequence/mutation database.

21. (Original) The computer system of claim 1, wherein the second database includes a genomic database.

22. (Original) The computer system of claim 1, wherein the records in the third database corresponding to biological information related to the chemical compounds effects on the biological targets, are organized in categories that include:

compound name;

target name;

toxicity;

side effects; and

mechanism of drug action.

23. (Original) The computer system of claim 1 further comprising means for setting an interaction test threshold corresponding to said effect and means for selecting the compound when its use results in a test meeting the interaction test threshold.

24. (Withdrawn) A method for analyzing data relevant to drug discovery and development comprising:

selecting chemical compounds from a first database containing records corresponding to a plurality of chemical compounds;

selecting molecular targets from a second database containing records corresponding to a plurality of molecular targets;

producing information corresponding to the interactions between each of the selected chemical compounds and each of the selected molecular targets;

selecting a biological activity from a third database containing records corresponding to biological information related to effects of chemical compounds on biological targets; and

using the produced information to correlate patterns of interactions between chemical compounds and molecular targets associated with the selected biological activity.

25. (Withdrawn) The method of claim 24, wherein the step of producing information includes the steps of

generating binding data of the binding between each of the selected chemical compounds and each of the selected molecular targets by monitoring the inhibitory effect that an unknown compound has on said binding;

setting a binding test threshold corresponding to the inhibitory effect; and generating information on the combination of unknown compound, molecular

target, and chemical compound that meets or fails to meet the binding test threshold.

26. (Withdrawn) The method of claim 25, wherein the binding data comprises positive and negative binding information.

27. (Previously Presented) The computer system of claim 1, wherein the interaction includes binding.

28. (Previously Presented) The computer system of claim 1, wherein the chemical compounds include compounds with known biological activity or that have failed in preclinical or human clinical tests.

29. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include compounds used in commerce as herbicides or pesticides.

30. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include known pharmaceuticals approved for human clinical use by the Food and Drug Administration.

31. (Withdrawn) The computer system of claim 1, wherein the molecular targets include ion channels.

32. (Withdrawn) The computer system of claim 1, wherein the molecular targets include transporters or uptake sites.

33. (Currently Amended) A computer system comprising:

a first database containing data corresponding to a plurality of chemical compounds;

a second database containing data corresponding to a plurality of molecular targets;

a third database containing data corresponding to screening results from *in vitro* assays measuring the interactions between each of a plurality of compounds in the first database and each of a plurality of molecular targets in the second database, the results including information on the effect that a compound selected from the first database has on the interaction between a reference compound known to interact with a selected molecular target from the second database and said selected molecular target; ~~and~~

a user interface allowing a user to ~~view information from the first database, the second database, and the third database as it relates to a compound record in the first database or as it relates to a molecular target in the second database or as it relates to one or more interaction records in the third database~~provide the system with information about a new chemical compound; and

a query script that extracts information from the three databases that is relevant to the predictability of the potential use of the new compound as a drug.

34. (Previously Presented) The computer system of claim 33, wherein the chemical compounds include compounds with known biological activity.

35. (Currently Amended) A computer system comprising:

a first database containing data corresponding to a plurality of chemical compounds and data corresponding to biological information related to effects of such chemical compounds on biological systems;

a second database containing data corresponding to a plurality of molecular targets;

a third database containing screening data corresponding to *in vitro* assays measuring interactions between each of a plurality of compounds in the first database and each of a plurality of molecular targets in the second database; ~~and~~

a user interface allowing a user to ~~view data from the first database, the second database, and the third database as it relates to at least one compound in the first database or as it relates to~~

~~at least one molecular target in the second database or as it relates to one or more interactions in the third database~~provide the system with information about a new chemical compound; and

a query script that extracts information from the three databases that is relevant to the predictability of the potential use of the new compound as a drug.

36. (Previously Presented) The computer system of claim 35, wherein the chemical compounds include compounds with known biological activity.

37. (Currently Amended) A computer system comprising:

a first database containing records corresponding to a plurality of chemical compounds and records corresponding to biological information related to effects of such chemical compounds on biological systems;

a second database containing records corresponding to a plurality of molecular targets; and

a third database containing records corresponding to screening results from *in vitro* assays measuring the interactions between each of a plurality of compounds in the first database and each of a plurality of molecular targets in the second database, the results including information on the effect that a compound selected from the first database has on the interaction between a reference compound known to interact with a selected molecular target from the second database and said selected molecular target; ~~and~~

a user interface that allows a user to ~~view information from at least one of the first database, the second database, and the third database~~provide the system with information about a new chemical compound; and

a query script that extracts information from the three databases that is relevant to the predictability of the potential use of the new compound as a drug.

38. (Previously Presented) The computer system of claim 37, wherein the user interface allows a user to view information from at least one of the first database, the second database, and the third database as it relates to a compound record in the first database.

39. (Previously Presented) The computer system of claim 37, wherein the user interface allows a user to view information from at least one of the first database, the second database, and the third database as it relates to a molecular target in the second database.

40. (Previously Presented) The computer system of claim 37, wherein the user interface allows a user to view information from at least one of the first database, the second database, and the third database as it relates to one or more interaction records in the third database.

41. (Previously Presented) The computer system of claim 37, wherein the interaction includes binding.

42. (Previously Presented) The computer system of claim 37, wherein the interaction includes binding and the effect includes inhibitory effect.

43. (Previously Presented) The computer system of claim 37, wherein the chemical compounds include compounds with known biological activity.

44 -57. (Canceled)

58. (Withdrawn) A system comprising: a memory including one or more data arrays of information associated with chemical compounds and molecular targets; and

a processor for executing a process for providing a user interface including: a representation of a selected chemical compound,

description information associated with the selected chemical compound, and biological information associated with the selected chemical compound.

59. (Currently Amended) A computer system comprising:

a first database containing records corresponding to a plurality of chemical compounds;

a second database containing records corresponding to a plurality of molecular targets;

a third database containing records corresponding to the screening results of *in vitro* assays to determine the interaction between each of a plurality of compounds in the first database and each of a plurality of targets in the second database, ~~and~~

a user interface allowing a user to ~~view data from the first database, the second database, and the third database as it relates to at least one compound in the first database or as it relates to at least one molecular target in the second database or as it relates to one or more interactions in the third database~~provide the system with information about a new chemical compound; and

a query script that extracts information from the three databases that is relevant to the predictability of the potential use of the new compound as a drug.

60. (Currently Amended) The computer system of claim 59, wherein the third database includes records corresponding to the results of ~~tests~~ *in vitro* assays to determine the interaction between all of the compounds selected to comprise a compound set in the first database and all of the molecular targets selected to comprise a molecular target set in the second database.

61. (Currently Amended) The computer system of claim 59, wherein the third database includes records corresponding to the results of *in vitro* assays ~~tests~~ to determine the interaction between a majority of the compounds selected to comprise a compound set in the first database and a majority of the molecular targets selected to comprise a molecular target set in the second database.

62. (Previously Presented) The computer system of claim 59, further comprising: a fourth database containing records corresponding to the effect of chemical compounds contained in the first database on biological systems.

63. (Currently Amended) The computer system of claim 62, wherein the third database includes records corresponding to the results of *in vitro* assays ~~tests~~ to determine the interaction between all of the compounds selected to comprise a compound set in the first

database and all of the molecular targets selected to comprise a molecular target set in the second database.

64. (Currently Amended) The computer system of claim 62, wherein the third database includes records corresponding to the results of *in vitro* assays ~~tests~~ to determine the interaction between a majority of the compounds selected to comprise a compound set in the first database and a majority of the molecular targets selected to comprise a molecular target set in the second database.

65. (Withdrawn) The computer system of claim 59, wherein the first database contains records corresponding to a plurality of known biologically active chemical compounds selected from among representatives of the following categories:

(a) pharmacological reference agents used in receptor, ion channel, transporter, or enzyme screening assays;

(b) drug candidates that have been approved by the Food and Drug Administration for testing in humans, including those that have been discontinued from further development; and

(c) pharmaceuticals that have been approved for human clinical use by the Food and Drug Administration, including those that have been subsequently withdrawn from the market.

66. (Withdrawn) The computer system of claim 65, wherein the known biologically active compounds included in the first database are further selected from among the following:

compounds that have been tested in preclinical studies in animals; pesticides;

herbicides;

bioactive natural products;

agricultural chemicals; and

environmental chemicals.

67. (Previously Presented) The computer system of claim 59, wherein the second database contains records corresponding to a plurality of molecular targets selected from among representatives of the following categories:

(a) receptors;

(b) ion channels;

(c) transporters; and

(d) enzymes.

68. (Currently Amended) The computer system of claim ~~65~~59, wherein the second database contains records corresponding to a plurality of molecular targets selected from among representatives of the following categories:

(a) receptors;

(b) ion channels;

(c) transporters; and

(d) enzymes.

69. (Withdrawn) The computer system of claim 67, wherein the molecular targets in the second database are related to drug discovery and development.

70. (Previously Presented) The computer system of claim 59, wherein the third database contains records corresponding to complete sets of results from a screening process.

71. (Currently Amended) The computer system of claim 59, wherein the records in the third database corresponding to the results of *in vitro* assays ~~tests~~ to determine the interaction between compounds in the first database and targets in the second database includes positive interactions and negative or lack of interactions.

72. (Currently Amended) The computer system of claim 59, wherein the *in vitro* assays ~~tests~~ to determine the interaction between compounds in the first database and the targets in the second database are based on binding interactions.

73. (Currently Amended) The computer system of claim 59, wherein the *in vitro* assays ~~tests~~ to determine the interaction between compounds in the first database and the targets

in the second database measure the inhibition of binding by a compound in the first database with respect to a target in the second database in the presence of another compound, such as a reference agent or enzyme substrate, known to interact with the target.

74. (Currently Amended) The computer system of claim 59, wherein the *in vitro* assays ~~tests~~ used to generate results comprising the third database are ligand binding assays.

75. (Currently Amended) The computer system of claim 59, wherein the *in vitro* assays ~~tests~~ used to generate results comprising the third database are enzyme inhibition assays.

76. (Currently Amended) The computer system of claim 59, wherein the *in vitro* assays ~~tests~~ to determine the interaction between compounds in the first database and the targets in the second database measure functional activity.

77. (Currently Amended) The computer system of claim 59, wherein the *in vitro* assays ~~tests~~ used to generate results comprising the third database measure adenyl cyclase activity, inositol triphosphate, or neurotransmitter transport.

78. (Currently Amended) The computer system of claim 59, wherein the *in vitro* assays ~~tests~~ used to generate results comprising the third database are based on reporter gene assays or functional assays.

79. (Currently Amended) The computer system of claim 59, wherein the results of *in vitro* assays ~~tests~~ to determine the interaction between compounds in the first database and targets in the second database are recorded in the third database as numerical values.

80. (Currently Amended) The computer system of claim 59, wherein the results of *in vitro* assays ~~tests~~ to determine the interaction between compounds in the first database and targets in the second database are recorded in the third database as per cent inhibition values.

81. (Currently Amended) The computer system of claim 59, wherein the results of *in vitro* assays ~~tests~~ to determine the interaction between compounds in the first database and targets in the second database are recorded in the third database as potency values.

82. (Currently Amended) The computer system of claim 59, wherein the results of *in vitro* assays ~~tests~~ to determine the interaction between compounds in the first database and targets in the second database are organized in the third database in terms of whether or not the interaction values exceed a specified threshold.

83. (Currently Amended) The computer system of claim 59, wherein the results of *in vitro* assays ~~tests~~ to determine the interaction between compounds in the first database and targets in the second database are organized in the third database in terms of whether or not the interaction values fall below a specified threshold.

84. (Currently Amended) The computer system of claim 59, wherein the results of *in vitro* assays ~~tests~~ to determine the interaction between compounds in the first database and targets in the second database are organized in the third database in terms of whether or not the interaction values fall between specified upper and lower thresholds.

85. (Currently Amended) The computer system of claim 59, wherein the results of *in vitro* assays ~~tests~~ to determine the interaction between compounds in the first database and targets in the second database are organized in the third database in terms of profiles of numerical values or meeting specified threshold criteria for specific compounds from the first database with respect to panels of molecular targets in the second database.

86. (Currently Amended) The computer system of claim 59, wherein the results of *in vitro* assays ~~tests~~ to determine the interaction between compounds in the first database and targets in the second database are organized in the third database in terms of profiles of numerical values or of meeting specified threshold criteria for specific compounds from the first database with respect to panels of molecular targets in the second database and in formats that

allow comparisons to be made (a) between such profiles among subsets of compounds in the first database or (b) between such profiles or groups of profiles of compounds in the first database and a comparable profile of interaction data for a compound or group of compounds not in the first database.

87. (Previously Presented) The computer system of claim 59, wherein the chemical compounds in the first database are selected from among the compound set comprising LOPAC (List Of Pharmacologically Active Compounds, Sigma/RBI).

88. (Previously Presented) The computer system of claim 59, wherein the chemical compounds in the first database are selected from among the compound set contained in United States Pharmacopeial Convention Inc.'s USP DI Series.

89. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include at least one of the following:

chemical name; chemical formula; chemical structure; molecular weight;
physical chemical properties;
chemical space coordinates;
chemical structural descriptors;
solubility; and
logP.

90. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include chemical structural descriptors that can be searched and analyzed using computer-based searching and data analysis methods.

91. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database are organized by chemical structural relatedness or as chemical descriptor arrays or tables.

92. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include chemical structural descriptors that can be analyzed using methods of recursive partitioning.

93. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include chemical structural descriptors that are organized in a format amenable to data analysis using CoMFA software or related methods.

94. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include chemical structural descriptors that are organized in a format amenable to data analysis using Catalyst/Hypo software or related methods.

95. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include SMILES codes.

96. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include 2-D topological descriptors.

97. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include 3-D pharmacophore descriptors.

98. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include substructure or chemical moiety descriptors.

99. (Previously Presented) The computer system of claim 59, wherein the first database also contains records corresponding to biological information related to effects of the chemical compounds on biological systems.

100. (Previously Presented) The computer system of claim 99, wherein the records in the first database corresponding to biological information includes information on chemical name, trade names, or alternative compound names and at least one of the following categories:

toxicity;

side effects;

mechanism of action; and

pharmacokinetics.

101. (Previously Presented) The computer system of claim 100, wherein records in the first database corresponding to biological information related to pharmacokinetic effects of selected chemical compounds on biological systems includes information on at least one of the following categories:

bioavailability;

absorption;

drug distribution;

drug metabolism;

drug excretion;

blood-protein binding; and blood-brain barrier passage.

102. (Previously Presented) The computer system of claim 100, wherein records in the first database corresponding to biological information related to toxicological effects of selected

chemical compounds on biological systems includes information on at least one of the following categories:

teratotoxicity;

mutagenicity; and

toxicity.

103. (Previously Presented) The computer system of claim 100, wherein records in the first database corresponding to biological information related to side effects of selected chemical compounds on biological systems includes information on at least one of the following categories:

known receptor interactions;

known enzyme interactions;

behavioral effect;

physiological effect; and

organ effects.

104. (Previously Presented) The computer system of claim 100, wherein records in the first database corresponding to biological information related to mechanism of action of selected chemical compounds on biological systems includes information on at least one of the following categories:

target organ;

major pathway;

minor pathway; and

putative molecular target for mode of action.

105. (Previously Presented) The computer system of claim 99, wherein records corresponding to biological information related to effects of the chemical compounds on biological systems can be searched and analyzed using computer-based searching and data analysis methods.

106. (Canceled)

107. (Previously Presented) The computer system of claim 99, wherein records corresponding to biological information related to effects of the chemical compounds on biological systems are encoded using numerical terms such as LD50, ED50, percent absorbed, half-life, and peak concentration.

108. (Previously Presented) The computer system of claim 59, wherein the targets in the second database are selected from among those comprising the superfamily of G-Protein Coupled Receptors, including the following types and subtypes: dopamine, serotonin, adrenergic, muscarinic/acetylcholine, histamine, adenosine, angiotensin, bradykinin, C5a, chemokine, CCK, endothelin, neuropeptide Y, neurotensin, opioid, somatostatin, tachykinin, vasopressin, galanin, prostanoid, cannabinoid, platelet-activating factor, thyrotropin releasing factor, leukotriene, corticotropin releasing factor, PACAP, vasoactive intestinal peptide, melatonin, glutamate, and GABA-B.

109. (Canceled)

110. (Previously Presented) The computer system of claim 59, wherein the targets in the second database are selected from among those non-steroidal or steroidal intracellular receptors, including estrogen, glucocorticoid, progesterone, and testosterone.

111. (Withdrawn) The computer system of claim 59, wherein the molecular targets in the second database comprise kinases or phosphatases.

112. (Withdrawn) The computer system of claim 59, wherein the molecular targets in the second database are selected from among those comprising cytochrome P450 enzymes.

113. (Withdrawn) The computer system of claim 59, wherein the molecular targets in the second database are selected from among those comprising DNA-modifying enzymes or transferases.

114. (Withdrawn) The computer system of claim 59, wherein the molecular targets in the second database are selected from among those comprising neurotransmitter-related enzymes.

115. (Withdrawn) The computer system of claim 59, wherein the molecular targets in the second database comprise proteases or carbohydrates.

116. (Withdrawn) The computer system of claim 69, wherein the molecular targets related to drug discovery and development include nucleic acids.

117. (Withdrawn) The computer system of claim 69, wherein the molecular targets related to drug discovery and development include carbohydrates.

118. (Withdrawn) The computer system of claim 59, wherein the molecular targets in the second database are selected from among sodium, potassium, calcium, chloride, or ligand-gated channels.

119. (Withdrawn) The computer system of claim 59, wherein the molecular targets in the second database are selected from among transporters or uptake sites for dopamine, serotonin, norepinephrine, adenosine, glycine, glutamate, and choline.

120. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database include at least one of the following: molecular target name;

molecular target family, classification or type;

corresponding gene DNA sequence;

amino acid sequence;

3-dimensional conformation or structure;

location of expression in tissues or cell types;

hydropathy plots; and

biochemical or molecular descriptors.

121. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized in a format amenable to computer-based searching and data analysis methods.

122. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by DNA sequence alignments.

123. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by DNA sequence homology.

124. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are grouped by family, superfamily, or subfamily.

125. (Currently Amended) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by species source of the molecular target used in the *in vitro* assay ~~test~~ to determine the interaction between chemicals and targets.

126. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by location of expression in tissues.

127. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by major or minor pathways.

128. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by distribution of molecular target protein expression across different cell types.

129. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by distribution of location of expression or across different cell types.

130. (Canceled)

131. (Canceled)

132. (Currently Amended) A computer system comprising:

a first database containing records corresponding to a plurality of chemical compounds,

a second database containing records corresponding to a plurality of molecular targets;

a third database containing records corresponding to the screening results of *in vitro* assays measuring the interaction between compounds in the first database and targets in the second database, wherein the third database includes records corresponding to the results of tests to determine the interaction between all possible combinations of the compounds selected to comprise a compound set in the first database and the molecular targets selected to comprise a molecular target set in the second database; ~~and~~

a user interface allowing a user to ~~view data from the first database, the second database, and the third database as it relates to at least one compound in the first database or as it relates to at least one molecular target in the second database or as it relates to one or more interactions in the third database~~provide the system with information about a new chemical compound; and

a query script that extracts information from the three databases that is relevant to the predictability of the potential use of the new compound as a drug.

133. (Canceled)

134 - 138. (Canceled)

139. (Currently Amended) A computer system comprising:

a first database containing records corresponding to a plurality of chemical compounds and records corresponding to biological information related to effects of such chemical compounds on biological systems;

a second database containing records corresponding to a plurality of molecular targets;

a third database containing records corresponding to screening results from *in vitro* assays measuring interactions between each of a plurality of compounds in the first database and each of a plurality of molecular targets in the second database, the results including information on the effect that a compound selected from the first database has on the interaction between a reference compound known to interact with a selected molecular target from the second database and said selected molecular target; ~~and~~

a user interface allowing a user to ~~view the selected compound and to selectively view information from the first database, the second database, and the third database as it relates to a compound record in the first database or as it relates to a molecular target in the second database,~~

~~wherein a process provides information reflecting a relationship between one or more compounds in the first database and one or more targets in the second database, the provided information being relevant to a predictability of a potential use of a new compound~~provide the system with information about a new chemical compound; and

a query script that extracts information from the three databases that is relevant to the predictability of the potential use of the new compound as a drug.

140. (Previously Presented) The computer system of claim 139, wherein the new relationship is provided to determine correlations that are useful for drug discovery and development.

141. (Previously Presented) The computer system of claim 139, wherein the relationship is provided to determine patterns that are useful for drug discovery and development.

142. (Currently Amended) A computer system comprising:

a first database containing records corresponding to a plurality of chemical compounds and records corresponding to biological information related to effects of such chemical compounds on biological systems, wherein the first database includes a database of chemical compounds that have failed in preclinical or human clinical tests;

a second database containing records corresponding to a plurality of molecular targets;

a third database containing records corresponding to *in vitro* assays measuring interactions between compounds in the first database and molecular targets in the second database, the results including information on the effect that a compound from the plurality of compounds has on the interaction of a compound known to interact with a molecular target from the plurality of molecular targets and said molecular target; ~~and~~

a user interface allowing a user to ~~view the selected compound and to selectively view information from the first database, the second database, and the third database as it relates to a compound record in the first database or as it relates to a molecular target in the second database~~provide the system with information about a new chemical compound; and

a query script that extracts information from the three databases that is relevant to the predictability of the potential use of the new compound as a drug.

143. (Canceled)

144. (Currently Amended) A computer system comprising:

a first database containing records corresponding to a plurality of chemical compounds, wherein the chemical compounds in the first database are selected from among the compound set contained in United States Pharmacopeial Convention Inc.'s USP DI Series;

a second database containing records corresponding to a plurality of molecular targets;

a third database containing records corresponding to the screening results of *in vitro* assays to determine the interaction between each of a plurality of compounds in the first database and each of a plurality of targets in the second database; ~~and~~

a user interface allowing a user to ~~view data from the first database, the second database, and the third database as it relates to at least one compound in the first database or as it relates to at least one molecular target in the second database or as it relates to one or more interactions in the third database~~provide the system with information about a new chemical compound; and

a query script that extracts information from the three databases that is relevant to the predictability of the potential use of the new compound as a drug.

145. (Currently Amended) A computer system comprising:

a first database containing records corresponding to a plurality of chemical compounds, wherein records corresponding to the chemical compounds in the first database include SMILES codes;

a second database containing records corresponding to a plurality of molecular targets;

a third database containing records corresponding to the screening results of *in vitro* assays to determine the interaction between each of a plurality of compounds in the first database and each of a plurality of targets in the second database; ~~and~~

a user interface allowing a user to ~~view data from the first database, the second database, and the third database as it relates to at least one compound in the first database or as it relates to at least one molecular target in the second database or as it relates to one or more interactions in the third database~~provide the system with information about a new chemical compound; and

a query script that extracts information from the three databases that is relevant to the predictability of the potential use of the new compound as a drug.